Multiscale Modeling of Forming and Fracture – Industry Perspective

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Advances in modeling deformation and fracture of granular materials at individual grain scales and their integration into component scale simulations using commercial codes have become enablers for implementing multiscale modeling schemes in the metal forming industry. Now it is possible to compute the forming limit diagram for aluminum sheet from electron backscattered diffraction data and simple tensile test data using crystal plasticity simulation at the grain scale, which can be coupled with anisotropic yield function modeling at a macroscale. The key to this advance has been the availability of new experimental and computational tools. Validation of model predictions with evolving microstructure data obtained through in situ multiaxial deformation tests at dislocation scale and electron backscatter diffraction scale have improved the confidence in constitutive models to capture the physics of deformation accurately. Parallel computing and meshless computing have enabled complex geometries, strain paths, crack tip deformation fields, etc. to be integrated efficiently in large component simulations. Among the benefits of this approach are (i) elimination of numerous and often difficult mechanical tests to calibrate anisotropic yield functions, (ii) ability to simulate evolving forming limit curves for smart forming strategies, and (iii) a microstructure-sensitive inverse design approach for materials development. Furthermore, the multiscale hierarchical approach allows for crystal plasticity model to be informed by lower length scale electronic and atomistic simulations of solute-dislocation interactions. Technological challenges such as eliminating negative strain rate sensitivity in Al-Mg alloys that is responsible for the PLC effect, serrations in room temperature tensile stress-strain curves and defects like stretcher marks on formed aluminum sheet panels can now be addressed through multiscale modeling. Details of the above applications will be presented along with a discussion of new challenges and opportunities in mutiscale modeling to enable an “atom to auto” approach in the future.

Quantitative study of the role of twin-parent and twin-twin interactions on the mechanical response of hexagonal materials

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Predicting the evolution of the macroscopic response and internal stress developments in metals necessitates the use of multi-scale approaches. In hexagonal material systems, this need is particularly exacerbated by the activation of twin modes, in addition to slip modes, which render the understanding microstructure evolutions and stress heterogeneity developments more complex. For example, the development of backstresses during twin growth remains partly unexplained and not captured by classical polycrystalline models.

The work to be presented aims at unraveling the role of twinning on the plastic response of hexagonal materials. The first part of the study is dedicated to quantifying the effect of twinning on internal stress development in hcp materials (i.e. Mg, Zr). The second part of the work aims at understanding the role of twin/twin interactions on the macroscopic response of materials.

In part 1, an eshelbian micromechanics approach based on the work of Tanaka and Mori is used to provide first in the elastic case, a relationship between twin morphology and internal stresses in both parent and twin domains. This approach is further extended to the case of elastoplasticity and the work is applied to the case of extruded AZ31 alloy. Prediction of the mechanical response and of average internal stress in the materials reveal the key role of the coupling between parent and twin phases in stress developments.

A second possible contributor to stress developments in hexagonals stems from the interaction between twin domains. Using a novel tool for pattern recognitions in EBSD maps of Zr and Mg, statistics of twin/twin interactions are obtained for different loading conditions. In particular the relative ratio of cozonal and non-cozonal interactions is shown. Atomistic studies are also used to probe the energy states in the loci of twin intersections. From these findings a new constitutive model is developed to predict the effect of latent interactions between twin domains in hcp polycyrtals.

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Direct and phase transformation-assisted grain reorientation in HCP titanium and BCC molybdenum

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Under severe plastic deformation, apart from popular plastic mechanisms, like dislocation, twinning, grain boundary sliding, grains in polycrystalline materials are reoriented to release stress rapidly. This is usually connected with unconventional processes. Using large-scale molecular dynamics simulations, we have investigated grain reorientation in titanium and molybdenum with the hexagonal close-packed and body-centered cubic structures, respectively. It is found that, in titanium direct grain reorientation occurs under certain unique combination of grain boundary and loading angle, while in molybdenum grain reorientation is achieved through phase transformation between body-centered and face-centered cubic structures. In this talk, the atomic details of such grain reorientation will be presented together with corresponding experimental confirmation.

A multi-scale model for transformation induced plasticity and the numerical calibration of its material parameters

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Transformation induced plasticity (TRIP) in martensitically transforming steels can be attributed to plasticity necessary to accommodate the lower density product phase on the one hand, and to an energetically favorable orientation of martensitic variants in the direction of the prevalent stress state on the other hand. In the proposed model these two effects are treated separately and accounted for by different strain contributions in their respective continuum mechanical description [1]. The effects related to the orientation of martensite variants is, for example, expressed in terms of an orientation strain whose evolution follows the classical framework of viscoplasticity. Experiments [2] indicate that dislocation controlled classical plasticity will only occur in the soft austenite parent phase while the orientation effect is limited to the martensite phase. It is thus necessary to resolve the given external stress state at the level of the individual phases using a scale transition rule as proposed by [3]. The parameters of the constitutive model for the constitutive equations as well as for the scale transition rule can partly be obtained from reference experiments. In addition, representative volume elements exemplarily representing the matrix – inclusion topology of the material in the course of transformation allow evaluating quantities, such as phase stresses, otherwise inaccessible to direct or indirect experimental observation.

The so calibrated material model also contains backstresses related to classical plasticity as well as to the orientation effect and is thus capable of predicting the material response even for non-proportional complex loading histories. Corresponding experiments prove the validity of the presented material model.

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A Mechanistic Study of Intergranular Cracking in Stainless Steels

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Intergranular cracks are known to initiate within heat affected zones of welded austenitic stainless steel components during service when reheated to the 500-700°C temperature range. In this work, the dominant mechanisms responsible for the nucleation of such grain boundary cracks are investigated experimentally and modelled numerically. An experimental procedure specially designed to reproduce the local conditions leading to intergranular cracking in 316L steels is followed. Here, a tensile residual stress field is introduced at the notch root of a CT specimen by deforming it at room temperature. It is then made to relax during thermal exposure at 550°C for a sufficiently long period of time so as to enable the nucleation of intergranular micro-cavities large enough to be observed by SEM, EBSD techniques and local X-ray tomography.

A novel visco-plastic constitutive material model is proposed to describe the mechanical behavior of the material under such reheat cracking conditions. The material model, formulated assuming large deformation kinematics, accounts for the microstructural evolution (dislocation density and mean twin spacing) and kinematic hardening during deformation through suitably defined internal variables. The model is calibrated from monotonic, cyclic and relaxation test data obtained between 20 and 600°C and is implemented numerically into the finite element method. It is then used to predict the generation of residual stress fields in the near-notch regions of the CT specimens during their pre-deformation at room temperature and their subsequent relaxation at 550-600°C. A good correlation is found between the distribution of the largest residual principal stress component predicted numerically and the experimentally observed intergranular damage.

In parallel to the residual stress predictions, which constitutes the main driving force for intergranular damage, the degradation of the inherent grain boundary properties due to the segregation of impurities such as phosphorus is studied. To that purpose, an existing phosphorus segregation kinetics model is used to predict the critical level of grain boundary phosphorus concentration at the moment when intergranular damage is detected experimentally. The results of this study have led to the development of a new alloy with a sufficiently low phosphorus content to avoid grain boundary embrittlement.

Linking Computational Stacking Fault Energies with Plasticity Mechanisms in High Temperature Carbide Ceramics

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Ceramics are often associated being hard and brittle, yet certain ceramics exhibit room temperature dislocation propagation as well as significant plasticity, upwards of 30%, at elevated temperature. Metal carbides are one such class of materials. However, due to their refractory nature, extensive testing at elevated temperatures can be prohibitive, which makes these systems particularly well suited for combined experimental and computational investigations to fully elucidate the deformation behavior. In this work, experiments, bending tests and indentation, with density functional theory calculations were combined to elucidate plastic deformation mechanisms. A series of TaC and Ta2C phases were either indented at room temperature or flexural tested near 2000 deg. C. Of these two phases, Ta2C exhibits more plasticity. The increase plasticity has been associated with a local metal-metal bond within the unit cell. This bond helps regulate both basal and non-basal slip, with experimentally determined slip quantified via dynamical electron diffraction. Experimental determined slip behavior was consistent with the density functional theory computed slip energy hierarchy. Additionally, the slip behavior between the rock salt group IV HfC and group V TaC is compared. Qualitatively, the TaC exhibited a higher density dislocation than HfC at all temperatures. {110} and {111} slip was observed in both systems, and its prevalence was observed as a function of temperature. The difference of slip plane is explained as differences in stable and unstable stacking fault energies between the two metal carbides.

A Multi-Scale Framework to Simulate Dynamic Recrystallization in Magnesium Alloys

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Warm/hot forming can increase the formability of magnesium alloys as this process increases the number of available slip systems due to thermal activation. When magnesium alloys are deformed at elevated temperatures, deformation is accommodated by slip and/or twinning until a critical value is reached. After this the material often exhibits dynamic recrystallization (DRX), which results in softening instead of hardening of the flow curve and can be detrimental or beneficial to Mg processing depending on the application. In this paper, a coupled approach to model DRX where the crystal plasticity based finite element (CPFEM) method is employed together with a probabilistic model to simulate both nucleation of a new grain and growth of the nucleus. The proposed numerical framework employs the local gradient in the dislocation density tensor in the deformed material to determine the nucleation of recrystallized grains. Furthermore, morphological aspects (length, width, etc.) of deformation twinning are introduced into the numerical analyses. This approach enforces equilibrium and compatibility between the twin zones and the parent matrix throughout the polycrystalline aggregate in the weak finite element sense. Twins are assumed to initiate at stress hot spots on the grain boundaries. These locations are then used as potential nucleation sites for DRX by neglecting any twin growth. Simulations of DRX are performed for AM30 and AZ31 magnesium alloys deformed at high temperatures and the predicted textures as well as the stress-strain curves are compared with experimental data to identify what further refinement of the model would improve accuracy.

Hierarchical multi-scale model: from texture and substructure to evolution of plastic anisotropy and complex hardening

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In this study we investigate how to incorporate micro-scale physical phenomena into simulations on a much larger length scale, such as modelling of sheet metal forming operations. Two important micro-scale processes interact during the plastic deformation: evolution of the crystallographic texture and evolution of the substructure. The two not only influence activity of deformation mechanisms, but also result in macroscopically observable changes in both plastic anisotropy and hardening. Furthermore, they are involved in cross-effects, such as hardening of different slip systems, which becomes critically important if the macroscopic deformation path is changed. From the macroscopic mechanical point of view, the hardening evolves substantially faster than the plastic anisotropy. For this reason it is even not uncommon to assume constant plastic anisotropy in simulations of metal forming processes, but the strain hardening is usually considered inconstant.

In this paper we propose a decoupling scheme that exploits the two disparate evolution rates to accelerate the multi-scale model of multi-step plastic deformation. In essence, we adopt a strategy of approximating outputs of a fine scale model that are relevant for a coarse scale model. To capture the evolution of the homogenized variables, the coarse scale model makes use of computationally inexpensive and short-living analytical approximations, which are adaptively reconstructed at different frequency.

Both the coarse-scale plastic anisotropy and the hardening are derived from a fine scale crystal plasticity (CP) model by means of virtual experiments. The CP considers the development of the intragranular dislocation substructure as well as the evolution of texture under the constraint of nearest neighbor grain-to-grain interaction. The plastic anisotropy at the coarse scale level is modelled by means of a plastic potential function, while the hardening is approximated and extrapolated by low order polynomial interpolation functions. Although a number of virtual experiments have to be conducted to construct the plastic potential function, it can be exploited by the coarse scale model for a relatively large range of macroscopic strain. On the other hand, the hardening model has to be updated more frequently, but the computational cost of an update is considerably lower. Moreover, the hardening can be extrapolated along a recent strain path, and the events of strain path change can be easily captured to trigger a necessary reconstruction of the approximation. We show that the hierarchical model is able to accurately simulate multi-stage deformation processes. The investigated case study consists of equibiaxial stretching followed by uniaxial tension, Bauschinger test and a deep drawing process that involves three subsequent changes of the deformation path.

Molecular Statics and Molecular Dynamics Simulations of Dislocation Behavior in a Model FCC Multicomponent Concentrated Solid Solution Alloy

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In this work, we explore developments in solid-solution alloys and study their application towards alloy discovery using atomistic simulations. Recent work shows that combining 4 or more elements in nearly equiatomic concentrations, may result in a unique class of single-phase materials having unusually high strengths. Similarly, recent developments in atomistic simulations shows that it may now be possible to simulate the behavior of such multicomponent alloys using interatomic potentials that allow one to mix atoms in any combination within a simulation. In this work, molecular statics and molecular dynamics simulations of a/2<110> screw and edge dislocation behavior for a model FCC $Ni_{30}Co_{30}Fe_{20}Ti_{20}$ alloy are discussed. The work shows that the single phase FCC lattice is elastically stable. Energies of selected points on the gamma surface for the model alloy are compared to that of pure Ni. The core structure a/2<110> screw and edge dislocations in the alloy are shown to be planar, having significant Shockley partial splitting variations along the dislocation line, resulting from concentration fluctuations. The critical stress to move both a/2<110> screw and edge dislocations at 0^{o}K is of the order of 0.005μ, where μ is the shear modulus, which is a value that is significantly ($\sim 10^{2}$) higher than that for pure FCC Ni. Molecular dynamics simulation results on the critical stress to move the a/2<110> screw and edge dislocations show that the critical stress decreases rapidly with increasing temperature, in a fashion that is similar to a BCC metal. These molecular dynamics simulation results are also shown to be in reasonable agreement with experimental tensile yield strength data for an analogous FCC alloy.